

THE THERMODYNAMIC PROPERTIES OF CUBANITE

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Introduction: CuFe_2S_3 exists in two polymorphs, a low-temperature orthorhombic form (cubanite) and a high-temperature cubic form (isocubanite) [e.g., 1]. Cubanite has been identified in the CI-chondrite and Stardust collections [2]. However, the thermodynamic properties of cubanite have neither been measured nor estimated. Our derivation of a thermodynamic model for cubanite allows constraints to be placed on the formation conditions. This data, along with the temperature constraint afforded by the crystal structure, can be used to assess the environments in which cubanite formation is (or is not) thermodynamically favored.

Methods: A thermodynamic model for cubanite was developed from measured heat capacity values for cubanite and isocubanite [3], entropy values for isocubanite [4], and the phase relationship between the 2 polymorphs. (Cubanite undergoes an irreversible phase transition to isocubanite at 210°C. Upon cooling below 210°C isocubanite does not revert to cubanite but rather exsolves chalcopyrite and pyrrhotite [e.g., 1].) From these data, entropy and enthalpy values were derived and used to estimate the Gibbs free energy of formation of cubanite.

The resultant thermodynamic data was used to explore the parameter space under which the formation of cubanite is thermodynamically favored. Aqueous processes and gas-solid corrosion processes were considered.

Results & Discussion: The derived thermodynamic values are consistent with: 1) the precipitation of cubanite from a CI-chondrite parent-body fluid in equilibrium with pyrrhotite, a process for which there is petrographic evidence [2, 5]; and 2) the precipitation of cubanite from a fluid in equilibrium with Cu metal, which is consistent with results from the experimental synthesis of cubanite under conditions relevant to the CI-chondrite parent body [6].

Cubanite's Gibbs free energy of formation is inconsistent with the formation of cubanite via corrosion of Cu and Fe metals by H_2S (g). Cubanite is both thermodynamically and kinetically inhibited from forming via nebular corrosion processes. To that end, cubanite has not been reported in any type 3 chondrites, which are most likely to retain signatures of nebular processes.

In lieu of the direct measurement of cubanite's thermodynamic properties, the derived estimates are a reasonable approximation, consistent with the meteoritic and experimental evidence.

Thermodynamic Properties of cubanite at 298.15K

C_p	S_T°	$\Delta_f H_T^\circ$	$\Delta_f G_T^\circ$	$\log K_f$
141.96	205.01	-278.04	-285.09	49.95
J/mole·K	J/mole·K	kJ/mole	kJ/mole	

References: [1] Cabri L. J. *et al.* 1973. *Can Min* 12:33-38. [2] Berger E. L. *et al.* 2011. *GCA* 75:3501-3513. [3] Sirota N. N. *et al.* 1985. *Doklady Akademii Nauk SSSR* 284:120-124. [4] Mizota T. *et al.* 1985. *Can Min* 23:77-82. [5] Bullock E. S. *et al.* 2005. *GCA* 69:2687-2700. [6] Berger E. L. *et al.* 2011. *MAPS Supplement*, id.5333.

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